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L4 2842848 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR AMIN? OR PROTEOME?)  
  
L5 224579 SEA FILE=HCAPLUS (MASS(W)SPECTR?)  
L6 26790 SEA FILE=HCAPLUS L4(L)L5  
L14 1924052 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR PROTEOME?)  
L27 1886 SEA FILE=HCAPLUS L14 (W)MASS  
L28 1074 SEA FILE=HCAPLUS L27 AND L6  
L30 436 SEA FILE=HCAPLUS L28 AND IDENT?  
L33 6258 SEA FILE=HCAPLUS L14(W)IDENT?  
L34 115 SEA FILE=HCAPLUS L30 AND L33  
L35 48 SEA FILE=HCAPLUS L34 NOT (2001 OR 2000 OR 1999)/PY

=> d ibib abs hitrn l35 1-48

L35 ANSWER 1 OF 48 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1999:3528 HCAPLUS  
DOCUMENT NUMBER: 130:150603  
TITLE: Examination of micro-tip reversed-phase liquid chromatographic extraction of **peptide** pools for **mass spectrometric** analysis  
AUTHOR(S): Erdjument-Bromage, Hediye; Lui, Mary; Lacomis, Lynne; Grewal, Anita; Annan, Roland S.; McNulty, Dean E.; Carr, Steven A.; Tempst, Paul  
CORPORATE SOURCE: Molecular Biology Program, Memorial Sloan-Kettering

Searched by Mona Smith phone: 308-3278

Page 1

SOURCE: Cancer Center, New York, NY, 10021, USA  
J. Chromatogr., A (1998), 826(2), 167-181  
CODEN: JCRAEY; ISSN: 0021-9673  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB **Mass spectrometry** occupies a central position in most current **protein identification** schemes. So-called 'mass fingerprinting' techniques rely on composite mass patterns of proteolytic fragments, or disson. products thereof, to query databases. Keys to successful anal. of ever smaller amts. are sensitivity and complete spectral information, both of which depend for a large part on proper sample prepn. Clean-up and concn. of **peptide** mixts. over Eppendorf gel loading tips filled with chromatog. media (i.e. 'micro-tips') are believed to be quite useful in this regard. We have studied quant. and qual. aspects of **polypeptide** extn. using these small manual devices. Optimization of sample vol. and additives, micro-tip bed vol., and eluent compn. and vol., all contribute to effective recovery (.apprx.65-70%, on av.). Improper digest conditions can, in fact, lead to far bigger losses, suggesting the need for at least trace amts. of Zwittergent 3-16. Of particular interest is our finding that partial fractionation, obtained by two-step micro-tip elution, generally results in more and better signals during subsequent mass anal. Thus, by using optimized micro-tips, in combination with adequate sample handling and instrumentation, direct **mass spectrometric identification** can be routinely and successfully done in any resource facility type setting.

## REFERENCE COUNT:

29

## REFERENCE(S):

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  - (7) Eng, J; J Am Soc Mass Spectrom 1994, V5, P976 HCAPLUS
  - (8) Erdjument-Bromage, H; Techniques in Protein Chemistry IV 1993, P419 HCAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 2 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:785231 HCAPLUS

DOCUMENT NUMBER: 130:121579

TITLE: **Mass spectrometric**

**identification** and microcharacterization of **proteins** from electrophoretic gels: strategies and applications

AUTHOR(S):

Jensen, Ole Norregaard; Larsen, Martin R.; Roepstorff, Peter

CORPORATE SOURCE:

Department of Molecular Biology, Odense University, Odense, Den.

SOURCE:

Proteins: Struct., Funct., Genet. (1998), (Suppl. 2), 74-89

PUBLISHER:

CODEN: PSFGEY; ISSN: 0887-3585  
Wiley-Liss, Inc.

DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review with 77 refs. including the authors' own research. The entire genomic DNA sequences of a no. of prokaryotic and eukaryotic species are now available and many more, including the human genome, will be completed in the near future. The state-of-life of a cell at any given time, however, is defined by its **protein compn.**, i.e., its **proteome**. Gel electrophoresis, **mass spectrometry**, and bioinformatics will be important tools for **protein and proteome anal.** in the post-genome era. **Protein identification** from electrophoretic gels by **mass spectrometric peptide mapping** or **peptide sequencing** combined with sequence database searching is established and has been applied to numerous biol. systems. We describe current strategies and selected applications in mol. and cell biol. The next challenges are detailed structure/function analyses, which include studying the mol. compn. of **multiprotein complexes** and characterization of secondary modifications of **proteins**. The advantages and limitations of a no. of **mass spectrometry**-based strategies designed for microcharacterization of low amts. of **protein** from electrophoretic gels are discussed and illustrated by examples.

REFERENCE COUNT: 79

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(4) Annan, R; Anal Chem 1996, V68, P3413 HCAPLUS  
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ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:704582 HCAPLUS

DOCUMENT NUMBER: 130:64992

TITLE: **Identification** of apoptosis-associated proteins in a human Burkitt lymphoma cell line. Cleavage of heterogeneous nuclear ribonucleoprotein A1 by caspase 3

AUTHOR(S): Brockstedt, Ekkehard; Rickers, Anke; Kostka, Susanne; Laubersheimer, Andreas; Dorken, Bernd; Wittmann-Liebold, Brigitte; Bommert, Kurt; Otto, Albrecht

CORPORATE SOURCE: Proteinchemie Max-Delbruck-Centrum fur Molekulare Medizin Humboldt University of Berlin, Robert Rossle Klinik, Berlin, D-13125, Germany

SOURCE: J. Biol. Chem. (1998), 273(43), 28057-28064  
CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Apoptosis or programmed cell death is essential in the process of controlling lymphocyte growth and selection. We **identified proteins** that are involved in anti-IgM antibody-mediated apoptosis

using a subclone of the human Burkitt lymphoma cell line BL60. Apoptosis-assocd. **proteins** were detected by high resohn. two-dimensional gel electrophoresis on a micropreparative scale. Comparison of the high resohn. two-dimensional gel electrophoresis **protein** patterns from apoptotic and non-apoptotic cells showed differences in .apprx.80 spots including **protein** modifications. Anal. of the predominantly altered **proteins** was performed by internal Edman microsequencing and/or by **peptide mass** fingerprinting using matrix-assisted laser desorption/ionization **mass spectrometry**. Anal. was significantly improved by using new micropreparative high resohn. two-dimensional gels employing high **protein** concns. The following 12 apoptosis-assocd. **proteins** were identified: heterogeneous nuclear **ribonucleoprotein** (hnRNP) A1, hnRNP C1/C2, FUSE-binding **protein**, dUTPase, lymphocyte-specific **protein** LSP1, UV excision repair **protein** RAD23 homolog B (HHR23B), 60 S acidic ribosomal **protein** P0 (L10E), heterochromatin **protein** 1 homolog .alpha. (HP1.alpha.), nucleolin, lamin, neutral calponin, and actin. Fragmentation of actin, hnRNP A1, hnRNP C1/C2, 60 S acidic ribosomal **protein** P0, lamin, and nucleolin could be inhibited by benzyloxycarbonyl-Asp(OMe)-Glu(OMe)-Val-Asp(OMe)-fluoromethyl ketone, a selective irreversible inhibitor of CPP32 (caspase 3).

REFERENCE COUNT: 44  
REFERENCE(S): (2) Bazar, L; Oncogene 1995, V10, P2229 HCAPLUS  
(3) Bharti, A; J Biol Chem 1996, V271, P1993 HCAPLUS  
(4) Boise, L; Science 1996, V274, P67 HCAPLUS  
(5) Cohen, G; Biochem J 1997, V326, P1 HCAPLUS  
(6) Dudley, B; J Biol Chem 1992, V267, P11964 HCAPLUS  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 4 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:697567 HCAPLUS  
DOCUMENT NUMBER: 130:63133  
TITLE: Microfabricated device coupled with an electrospray ionization quadrupole time-of-flight **mass spectrometer: protein identifications** based on enhanced-resolution **mass spectrometry** and tandem **mass spectrometry** data  
AUTHOR(S): Figeys, Daniel; Lock, Chris; Taylor, Lorne; Aebersold, Ruedi  
CORPORATE SOURCE: Institute for Marine Biosciences, National Research Council Canada, Halifax, NS, Can.  
SOURCE: Rapid Commun. Mass Spectrom. (1998), 12(20), 1435-1444  
CODEN: RCMSEF; ISSN: 0951-4198  
PUBLISHER: John Wiley & Sons Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB We describe the coupling of a microfabricated fluidic device to an electrospray ionization (ESI) quadrupole time-of-flight **mass spectrometer** (QqTOFMS) for the **identification** of **protein** samples. The microfabricated devices consisted of three reservoirs connected via channels to a main capillary, which in turn was linked via a microspray interface to the QqTOFMS. Here we present

preliminary results obtained using this system. Standardized solns. of myoglobin tryptic digest were analyzed indicating a limit of detection at the low to sub fmol/pLL. The combination of the microfabricated device for rapid sample delivery and the rapid acquisition capability, enhanced resoln. and mass accuracy of the QqTOF offers unique possibilities for the rapid **identification of proteins** by database searching. This platform can generate MS data suitable for **protein** database searching by the **peptide-mass** fingerprinting approach and MS/MS data suitable for **protein** database searching. Here the results of the two database-searching approaches are compared and the possibilities of combining the two approaches for rapid **identification of protein** are discussed. Also, we present a comparison of the results obtained using the three-position microfabricated device coupled to the ESI-QqTOFMS and to an ESI-ion trap MS. Finally the combination of C-terminal 180 labeling of **peptides** and the microfabricated system for automated combined **peptide-mass** fingerprinting and sequence-tag database searching is discussed.

REFERENCE COUNT: 42  
REFERENCE(S): (2) Betts, J; J Biol Chem 1997, V272, P12922 HCAPLUS  
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ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 5 OF 48 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1998:686618 HCAPLUS  
DOCUMENT NUMBER: 130:49374  
TITLE: Characterization of Serine and Threonine  
Phosphorylation Sites in .beta.-  
Elimination/Ethanethiol Addition-Modified  
**Proteins** by Electrospray Tandem Mass  
**Spectrometry** and Database Searching  
AUTHOR(S): Jaffe, Howard; Veeranna; Pant, Harish C.  
CORPORATE SOURCE: LNC-NINDS Protein/Peptide Sequencing Facility National  
Institute of Neurological Disorders and Stroke,  
National Institutes of Health, Bethesda, MD, 20892,  
USA  
SOURCE: Biochemistry (1998), 37(46), 16211-16224  
CODEN: BICHAW; ISSN: 0006-2960  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A new method for the characterization of serine and threonine  
phosphorylation sites in **proteins** has been developed. After  
modification of a **phosphoprotein** by .beta.-  
elimination/ethanethiol addn. and conversion of phosphoserine and  
phosphothreonine residues to S-ethylcysteinyl or .beta.-methyl-S-  
ethylcysteinyl residues, the modified **protein** was subjected to  
proteolytic digestion. Resulting digests were analyzed by a combination  
of microbore liq. chromatog., electrospray ionization tandem (MS/MS) ion

trap mass spectrometry and database searching to identify original phosphorylated residues. The computer program utilized (SEQUEST) is capable of identifying peptides and modified residues from uninterpreted MS/MS spectra, and using this method, all of the five known phosphorylation sites in bovine .beta.-casein were identified. Application of the method to multiply phosphorylated human high mol. wt. neurofilament protein (NF-H) resulted in the identification of 21 peptides and their modified residues and hence, the in vivo phosphorylation sites. These included 26 KSP and 1 KTP site, all of which occur in the KSP repeat C-terminal tail domain (residues 502-823). One site at residue 518 was previously uncharacterized. A novel non-KSP serine at residue 421 near the KLLGEE region in a IPFSLPE motif was characterized as phosphorylated (or glycosylated). The 27 characterized phosphorylation sites occur at S/TP residues in the following motifs: KSPVKEE, KSPAEEK, KSPEKEE, KSPAENV, KSPEKAK, KSPPEAK, KSPVKAEE, and KTPAKEE. On the basis of kinase consensus sequences, all of these motifs, including the previously unreported KTPAKEE motif, can be phosphorylated by proline-directed kinases. Advantages of the new method vis-a-vis our previously reported method [Jaffe, H., Veeranna, Shetty, K. T., and Pant, H. C. (1998) Biochem. 37, 3931-3940] include (i) prodn. of diastereomers eluting at different retention times increased the chances of peptide identification, (ii) increased hydrophobicity and hence retention time of the modified peptides, (iii) facilitation of pos. ion prodn., and (i.v.) increased susceptibility to tryptic digestion as a result of conversion of neg. charged phosphorylated residues to neutral S-ethylcysteine or .beta.-methyl-S-ethylcysteine residues.

## REFERENCE COUNT:

43

## REFERENCE(S):

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  - (5) Bennett, G; J Neurochem 1997, V68, P534 HCAPLUS
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- ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 6 OF 48 HCAPLUS COPYRIGHT 2001 ACS

## ACCESSION NUMBER:

1998:635863 HCAPLUS

## DOCUMENT NUMBER:

129:341417

## TITLE:

Towards an automated approach for protein identification in proteome projects

## AUTHOR(S):

Traini, Mathew; Gooley, Andrew A.; Ou, Keli; Wilkins, Marc R.; Tonella, Luisa; Sanchez, Jean-Charles; Hochstrasser, Denis F.; Williams, Keith L.

## CORPORATE SOURCE:

Center Analytical Biotechnology, School Biological Sciences, Macquarie University, Sydney, 2109, Australia

## SOURCE:

Electrophoresis (1998), 19(11), 1941-1949  
CODEN: ELCTDN; ISSN: 0173-0835

## PUBLISHER:

Wiley-VCH Verlag GmbH

## DOCUMENT TYPE:

Journal

## LANGUAGE:

English

AB The development of automated, high throughput technologies for the rapid identification of proteins is essential for large-scale proteome projects. While a degree of automation already exists in

some stages of the **protein identification** process, such as automated acquisition of matrix assisted laser desorption ionization-time of flight (MALDI-TOF) **mass spectra**, efficient interfaces between different stages are still lacking. The authors report the development of a highly automated, integrated system for large scale **identification of proteins** sepd. by 2-D gel electrophoresis, based on **peptide mass** fingerprinting. A prototype robotic system was used to image and excise 288 **protein spots** from an amido black stained polyvinylidene difluoride (PVDF) blot. **Protein** samples were enzymically digested with a com. automated liq. handling system. MALDI-TOF **mass spectrometry** was used to acquire **mass spectra** automatically, and the data analyzed with novel automated **peptide mass** fingerprinting database interrogation software. Using this highly automated system, the authors were able to **identify 95 proteins** on the basis of **peptide mass** fingerprinting, isoelec. point and mol. wt., in a period of less than 10 working days. Advantages, problems, and future developments in robotic excision systems, liq. handling, and automated database interrogation software are discussed.

L35 ANSWER 7 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:635861 HCAPLUS

DOCUMENT NUMBER: 129:341416

TITLE: **Identification of yeast proteins from two-dimensional gels. Working out spot cross-contamination**

AUTHOR(S): Parker, Kenneth C.; Garrels, James I.; Hines, Wade; Butler, Erin M.; McKee, Andrew H. Z.; Patterson, Dale; Martin, Steve

CORPORATE SOURCE: PerSeptive Biosystems, Framingham, MA, 01701, USA

SOURCE: Electrophoresis (1998), 19(11), 1920-1932

CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB With the complete sequence of the yeast genome now available, efforts by many labs. are underway to **identify** each of the spots on 2-D gels corresponding to the most abundant yeast **proteins**. The high mass accuracy now attainable using matrix assisted laser desorption/ionization (MALDI)-**mass spectrometry** equipped with delayed extn. simplifies the process of **identification**, such that many spots can be unambiguously **identified** in a short period of time merely by **peptide mass** fingerprinting and generally available database matching programs. Although it is not always possible to match spots between gels run by different labs., **proteins** generally yield the same abundant proteolytic fragments when tryptic digestions are performed. Databases contg. these signature **peptides** not only simplify the task of reidentifying **proteins** from different gels, but also make it possible to **identify** small amts. of cross-contaminating **proteins** from different spots, as well as common extraneous contaminants such as human keratins. The authors present data on the **identification of >20 previously unreported yeast proteins**

from 2-D gels. Some novel **proteins** were **identified** from randomly analyzed spots. Focusing on 14 spots in a narrow-pH-range gel, the authors demonstrate how organizing peak-table data and **peptide** match-list data into databases enables the **identification** of a larger % of the peaks.

L35 ANSWER 8 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:386801 HCAPLUS

DOCUMENT NUMBER: 129:51685

TITLE: Two-dimensional electrophoresis of human placental mitochondria and **protein identification by mass spectrometry**. Toward a human mitochondrial **proteome**

AUTHOR(S): Rabilloud, Thierry; Kieffer, Sylvie; Procaccio, Vencent; Louwagie, Mathilde; Courchesne, Paul L.; Patterson, Scott D.; Martinez, Pascal; Garin, Jerome; Lunardi, Joel

CORPORATE SOURCE: CEA-Lab. BioEnergetique Cellulaire Pathologique, Grenoble, F-38054, Fr.

SOURCE: Electrophoresis (1998), 19(6), 1006-1014  
CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Owing to the complexity of higher eukaryotic cells, characterization of a complete proteome is likely to be difficult to achieve. Advantage can be taken of the cell compartmentalization to build organelle proteomes, which can moreover be viewed as specialized tools to study specifically the biol. and "physiol." of the target organelle. Within this frame, the authors report here the construction of the human mitochondrial proteome, using placenta as the source tissue. **Protein identification** was carried out mainly by **peptide mass** fingerprinting, but other methods were also used (N-terminal microsequencing, blotting). The optimization steps in 2-dimensional (2-D) electrophoresis needed for proteome research are discussed. The relative paucity of data concerning mitochondrial proteins is still the major limiting factor in building the corresponding proteome, which should be a useful tool for researchers working on human mitochondria and their deficiencies.

L35 ANSWER 9 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:386799 HCAPLUS

DOCUMENT NUMBER: 129:105694

TITLE: The **identification** of peptide modifications derived from gel-separated proteins using electrospray triple quadrupole and ion trap analyses

AUTHOR(S): Swiderek, Kristine M.; Davis, Michael T.; Lee, Terry D.

CORPORATE SOURCE: Beckman Research Inst., City Hope, Duarte, CA, USA

SOURCE: Electrophoresis (1998), 19(6), 989-997

CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal



LANGUAGE: English

AB Microspray tandem **mass spectrometry** (MS/MS) in combination with database search routines has become a powerful tool for the **identification** of **proteins** from femtomole amts. of material following gel electrophoresis and in-gel digestion procedures. Artifactual modification of susceptible residues can arise during gel electrophoresis, leading to unexpected **peptide mass** shifts during mass anal. Collision-induced dissocn. (CID) spectra generated from these derivatized **peptides** can defy direct interpretation by automated database search routines and remain unidentified. The authors evaluate the MS/MS spectra of **peptides** carrying oxidized derivs. of Trp and Met residues, and various modifications of Cys. The authors demonstrate that certain of these modifications generate characteristic fragmentation patterns or "fingerprints", during CID anal., the knowledge of which can facilitate the interpretation of the spectra. The authors show that these signature fragment ions are predominantly produced during the CID anal. of singly charged ions although they can be obsd. in the MS/MS spectra of the doubly charged species as well. In other cases, the CID spectrum lacks a characteristic fingerprint and the modification remains silent. CID spectra of related **peptides**, differing only by their modifications, are similar and all or part of the fragment ion spectra will have shifted by a discreet mass, which facilitates the **identification** of the modified residue. At the same time, the comparison of related spectra can prevent misinterpretations such as the assignment of a residue mass to the wrong **amino acid** or a neutral loss fragment ion to a y- or b-ion.

L35 ANSWER 10 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:386797 HCAPLUS

DOCUMENT NUMBER: 129:51121

TITLE: Rapid **identification** of comigrating gel-isolated **proteins** by ion trap-**mass spectrometry**

AUTHOR(S): Arnott, David; Henzel, William J.; Stults, John T.

CORPORATE SOURCE: Protein Chem. Dep., Genentech Inc., San Francisco, CA, 94080, USA

SOURCE: Electrophoresis (1998), 19(6), 968-980

CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the search for novel nuclear binding **proteins**, 2 bands from a Na dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) gel were analyzed and each was found to contain a no. of **proteins** that subsequently were **identified** by tandem **mass spectrometry** (MS/MS) on a quadrupole ion trap instrument. The bands were digested with trypsin in situ on a polyvinylidene difluoride (PVDF) membrane following electroblot transfer. Anal. of a 2.5% aliquot of each **peptide** mixt. by matrix assisted laser desorption/ionization-**mass spectrometry** (MALDI-MS) followed by an initial database search with the **peptide** masses failed to **identify** the **proteins**. The **peptides** were sepd. by reversed-phase capillary HPLC in anticipation of subsequent Edman

degrdn., but mass anal. of the chromatog. fractions by MALDI-MS revealed multiple, coeluting **peptides** that precluded this approach. Selected fractions were analyzed by capillary HPLC-electrospray ionization-ion trap **mass spectrometry**. Tandem **mass spectrometry** provided significant fragmentation from which full or partial sequence was deduced for a no. of **peptides**. 2 Stages of fragmentation by multistage **mass spectrometry** were used in a case to det. addnl. sequence. Database searches, each using a single **peptide mass** plus partial sequence, **identified 4 proteins** from a single electrophoretic band at 45 kDa, and 4 **proteins** from a 2nd band at 60 kDa. Many of these **proteins** were derived from human keratin. The **protein identifications** were corroborated by the presence of multiple matching **peptide masses** in the MALDI-MS spectra. A novel sequence, not found in **protein** or DNA databases, was detd. by interpretation of the MS/MS data. These results demonstrate the power of the quadrupole ion trap for the **identification** of multiple **proteins** in a mixt., and for de novo detn. of **peptide** sequence. Reanal. of the fragmentation data with a modified database searching algorithm showed that the same sets of **proteins** were **identified** from a limited no. of fragment ion masses, in the absence of **mass spectral** interpretation or **amino acid** sequence. The implications for **protein identification** solely from fragment ion masses are discussed, including advantages for low signal levels, for a redn. of the necessary interpretation expertise, and for increased speed.

L35 ANSWER 11 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:386796 HCAPLUS

DOCUMENT NUMBER: 129:51120

TITLE: Optimization of capillary chromatography ion trap-  
**mass spectrometry** for  
**identification** of gel-separated  
**proteins**

AUTHOR(S): Courchesne, Paul L.; Jones, Michael D.; Robinson, John  
H.; Spahr, Chris S.; McCracken, Susan; Bentley, David  
L.; Luethy, Roland; Patterson, Scott D.  
CORPORATE SOURCE: Amgen Center, Amgen Inc., Thousand Oaks, CA, 91320,  
USA

SOURCE: Electrophoresis (1998), 19(6), 956-967

CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The current paradigm for **protein identification** using  
**mass spectrometric** derived **peptide-**  
**mass** and fragment-ion data employs computer algorithms which match  
uninterpreted or partially interpreted fragment-ion data to sequence  
databases, both **protein** and translated nucleotide sequence  
databases. Nucleotide sequence databases continue to grow at a rapid rate  
for some species, providing an unsurpassed resource for **protein**  
**identification** in those species. Ion-trap **mass**  
**spectrometers** with their ability to rapidly generate fragment-ion  
spectra in a data-dependent manner with high sensitivity and accuracy has

led to their increased use for **protein identification**. The authors have investigated various parameters on a com. ion trap-**mass spectrometer** to enhance the ability to **identify peptides** sepd. by capillary reversed phase-high performance liq. chromatog. (RP-HPLC) coupled online to the **mass spectrometer**. By systematically evaluating the std. parameters (ion injection time and no. of microscans) together with selection of multiple ions from the full mass range, improved tandem **mass spectrometry** (MS/MS) spectra were generated, facilitating **identification of proteins** at a low pmol level. Application of this technol. to the **identification** of a std. **protein** and an unknown from an affinity-enriched mixt. are shown.

L35 ANSWER 12 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:386795 HCAPLUS

DOCUMENT NUMBER: 129:51119

TITLE: Capillary column chromatography improves sample preparation for mass spectrometric analysis. Complete characterization of human .alpha.-enolase from tow-dimensional gels following in situ proteolytic digestion

AUTHOR(S): Reid, Gavin E.; Rasmussen, Richele K.; Dorow, Donna S.; Simpson, Richard J.

CORPORATE SOURCE: Joint Protein Structure Lab., Ludwig Inst. Cancer Research, Royal Melbourne Hospital, Parkville, 3050, Australia

SOURCE: Electrophoresis (1998), 19(6), 946-955

CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors evaluate capillary column RP-HPLC/**mass spectrometric** approaches for **identifying** and characterizing 2-DE resolved **proteins**. Stable and efficient 0.20 mm and 0.32 mm internal diam. (ID) fused-silica columns with hydrophilic polyvinylidene difluoride (PVDF) frits were fabricated and slurry packed with 7 .mu.m spherical, 300 A pore size, C8 bonded phase silica particles. The authors show that capillary column chromatog. is a rapid and efficient desalting/ concg. (ON/OFF) technique for sample cleanup prior to **protein identification** by **peptide-mass** fingerprinting using matrix-assisted laser desorption ionization (MALDI)-time-of-flight **mass spectrometry**. While marginally more **peptide mass** information can be obtained by stepped elution of the **peptide** mixt. with increasing concns. of org. solvent, best results were obtained by fractionation of the **peptide** mixt. using a linear 60 min gradient. A salient feature was the observation that, in contrast to the stepped elution and gradient approaches, the ionization of **peptide** T1 (m/z 2402.2 SGETEDTFIADLVV(PeCys)TGQIK) was almost completely suppressed using the ON/OFF approach. Maximal **amino acid** sequence coverage, a necessary prerequisite for complete characterization of a **protein**, was accomplished using a capillary column (0.2 mm ID) directly coupled with an electrospray ionization (ESI) ion-trap tandem **mass spectrometer**.

For example, from an in situ tryptic digest of .alpha.-enolase isolated by 2-DE from the human breast carcinoma cell line MDA-MB231, 71% of the **amino** acid sequence was obtained. In addn. to **identifying** 2 possible N-terminal acetylated .alpha.-enolase variants, Asn153Asp and Ile152Asp/Asn153Ile, the tandem **mass spectrometric** data revealed the presence of a no. of process-induced modifications of .alpha.-enolase such as Met oxidn. and Cys amidoethylation.

L35 ANSWER 13 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:386789 HCAPLUS  
DOCUMENT NUMBER: 129:14031  
TITLE: Database searching using mass spectrometry data  
AUTHOR(S): Yates, John R., III  
CORPORATE SOURCE: Dep. Molecular Biotechnol., Univ. Washington, Seattle, WA, 98185, USA  
SOURCE: Electrophoresis (1998), 19(6), 893-900  
CODEN: ELCTDN; ISSN: 0173-0835  
PUBLISHER: Wiley-VCH Verlag GmbH  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review with 48 refs. Large-scale DNA sequencing is creating a sequence infrastructure of great benefit to **protein** biochem. Concurrent with the application of large-scale DNA sequencing to whole genome anal., **mass spectrometry** has attained the capability to rapidly, and with remarkable sensitivity, det. wts. and **amino** acid sequences of **peptides**. Computer algorithms were developed to use the 2 different types of data generated by **mass spectrometers** to search sequence databases. When a **protein** is digested with a site-specific protease, the mol. wts. of the resulting collection of **peptides**, the mass map or fingerprint, can be detd. using **mass spectrometry**. The mol. wts. of the set of **peptides** derived from the digestion of a **protein** can then be used to **identify** the **protein**. Several different approaches were developed. **Protein identification using peptide mass mapping** is an effective technique when studying organisms with completed genomes. A 2nd method is based on the use of data created by tandem **mass spectrometers**. Tandem **mass spectra** contain highly specific information in the fragmentation pattern as well as sequence information. This information was used to search databases of translated **protein** sequences as well as nucleotide databases such as expressed sequence tag (EST) sequences. The ability to search nucleotide databases is an advantage when analyzing data obtained from organisms whose genomes are not yet completed, but a large amt. of expressed gene sequence is available (e.g., human and mouse). Furthermore, a strength of using tandem **mass spectra** to search databases is the ability to **identify proteins** present in fairly complex mixts.

L35 ANSWER 14 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:350386 HCAPLUS  
DOCUMENT NUMBER: 129:78616  
TITLE: **Mass spectrometry of peptides in neuroscience**

AUTHOR(S): Nilsson, Carol L.; Karlsson, Gosta; Bergquist, Jonas;  
Westman, Ann; Ekman, Rolf  
CORPORATE SOURCE: Institute of Clinical Neuroscience, Department of  
Psychiatry and Neurochemistry, Sahlgrenska University  
Hospital/Molndal, Goteborg University, Moelndal,  
S-431, Swed.  
SOURCE: Peptides (N. Y.) (1998), 19(4), 781-789  
CODEN: PPTDD5; ISSN: 0196-9781  
PUBLISHER: Elsevier Science Inc.  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review with 53 refs. focuses on the contributions of modern **mass spectrometry** to **neuropeptide** research. An introduction to newer **mass spectrometric** techniques is provided. Also, the use of **mass spectrometry** in combination with high-resoln. sepn. techniques for **neuropeptide identification** in biol. samples is illustrated. The **amino acid** sequence information that is important for the **identification** and anal. of known, novel, or chem. modified **neuropeptides** may be obtained using **mass spectrometric** techniques. Because **mass spectrometry** techniques can be used to reflect the dynamic properties assocd. with **neuropeptide** processing in biol. systems, they may be used in the future to monitor **peptide** profiles within organisms in response to environmental challenges such as disease and stress.

L35 ANSWER 15 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:75036 HCAPLUS  
DOCUMENT NUMBER: 128:189941  
TITLE: **Mass spectrometry** and the age of  
the **proteome**  
AUTHOR(S): Yates, John R., III  
CORPORATE SOURCE: Department of Molecular Biotechnology, School of  
Medicine, University of Washington, Seattle, WA,  
98195-7730, USA  
SOURCE: J. Mass Spectrom. (1998), 33(1), 1-19  
CODEN: JMSPFJ; ISSN: 1076-5174  
PUBLISHER: John Wiley & Sons Ltd.  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review with 136 refs. **Mass spectrometry** has become an important technique to correlate **proteins** to their genes. This has been achieved, in part, by improvements in ionization and mass anal. techniques concurrently with large-scale DNA sequencing of whole genomes. Genome sequence information has provided a convenient and powerful resource for **protein identification** using data produced by matrix-assisted laser desorption/ionization time-of-flight (MALDI/TOF) and tandem **mass spectrometers**. Both of these approaches have been applied to the **identification** of electrophoretically sepd. **protein** mixts. New methods for the direct **identification** of **proteins** in mixts. using a combination of enzymic proteolysis, liq. chromatog. sepn., tandem **mass spectrometry** and computer algorithms which match **peptide** tandem **mass**

**spectra** to sequences in the database are also emerging. This tutorial review describes the principles of ionization and mass anal. for **peptide** and **protein** anal. and then focuses on current methods employing MALDI and electrospray ionization for **protein identification** and sequencing. Database searching approaches to **identify proteins** using data produced by MALDI/TOF and tandem **mass spectrometry** are also discussed.

L35 ANSWER 16 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:797221 HCAPLUS

DOCUMENT NUMBER: 128:112425

TITLE: **Protein identification** from 2-DE gels by MALDI **mass spectrometry**

AUTHOR(S): Jungblut, Peter; Thiede, Bernd

CORPORATE SOURCE: Proteinanalysis, Max-Planck-Institute for Infectionbiology, Berlin, D-10117, Germany

SOURCE: Mass Spectrom. Rev. (1997), 16(3), 145-162

CODEN: MSRVD3; ISSN: 0277-7037

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 149 refs. Two-dimensional electrophoresis (2-DE) allows the sepn. of **proteins** at the level of **protein** species, which are defined by their chem. structure. Each chem. modification leads to a new **protein** species. Prerequisites for investigations of **protein** species are reproducible sample prepn., large gels (20 .times. 30 cm and larger), high sensitive detection methods, automated evaluation of gels, and sensitive methods for **identification** of 2-DE-sepd. **protein** species. MALDI **mass spectrometry** with its sensitivity in the fmol range fits with the sensitivity of **protein** detection on 2-De gels. **Protein mass** detn., **peptide mass** mapping, post-source decay sequencing, and ladder sequencing by MALDI-MS in combination with genome databases have the potential for complete structural investigation on the **protein** species level. The discrimination of 19 cryst. species of mouse eye lens and of 54 human heart heat-shock **protein** 27 species shows the capacity of the combination of 2-DE with MALDI-MS.

L35 ANSWER 17 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:741808 HCAPLUS

DOCUMENT NUMBER: 128:84831

TITLE: Development of carboxyl-terminal sequencing methods for **proteins** and **peptide** by the use of FAB **mass spectrometry** and perfluoric acid

AUTHOR(S): Tsugita, Akira

CORPORATE SOURCE: Research Institute for Biosciences, Science University of Tokyo, Noda, 278, Japan

SOURCE: J. Mass Spectrom. Soc. Jpn. (1997), 45(5), 561-589

CODEN: JMSJEY; ISSN: 1340-8097

PUBLISHER: Nippon Shitsuryo Bunseki Gakkai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB We have developed the following unique methods essentially for carboxyl

(C)-terminal sequencing of proteins and peptides. The first and important observation was the successive truncation reaction of peptide with the use of 90% pentafluoropropionic acid (PFPA) and heptafluorobutyric acid (HFBA) at 90.degree.C for 4-24 h by FAB and ESI-MS. This observation indicated two informations, one of which was the reaction-intermediate to be the prediction of the oxazolones at resp. carboxyl termini of the truncated fragments, and the other was internal bond specific cleavages of carboxyl side of aspartic acid residue (Asp-C) and amino side of serine residue (Ser-N) as the side-reactions. The formation of oxazolone promoted using perfluorate anhydride. The extensive successive truncation was also carried out even at -20.degree.C within 1 h by the use of the perfluorate anhydride in acetonitrile soln. The side reactions, Asp-C and Ser-N were further studied; 0.2% PFPA aq. vapor at 60.degree.C for 24 h selectively cleaved ASP-Pro bond (60.degree.C, h) and the same acid vapor at 90.degree.C for 4-8 h cleaved Asp-C. An aq. 90% PFPA vapor at 25.degree.C for 48 h made N-O peptidyl shift at Ser/Thr. This was reacted with a vapor of 20% acetic anhydride and 1% acetic acid in acetoritrile at 60.degree.C for 1 h. The reaction acetylated the free NH<sub>2</sub>-groups of the Ser/Thr and the shifted peptide fragments. And finally 20% pimethylaminoethanol (DMAE) aq. soln. at 60.degree.C for 30 min cleaved the O-ester peptide fragment off from OH-group of Ser/Thr residue. These two specific cleavages can be used for **protein-identification** by the aid of "**peptide mass databases**" made from protein sequence database. The successive truncation accompanied by Asp-C or Ser-N cleavages with 90% PFPA at 90.degree.C for 1, 2, 4, and 8 h yielded multi-C-terminal sequences of protein. The data of several residues at several sites in protein provided information for **protein identification** again as well for general gene technol. In the last two methodologies TOF-MS and FAB-MS were efficiently employed. A step wise C-terminal sequence method has been developed from the successive truncation reactions, which composed of the following three reactions: (1) formation of oxazolone and acetylation of the N-terminus with a vapor of acetic anhydride with 10% acetic acid at 60.degree.C for 1 h; (2) cleavage off the C-terminal amino acid from the oxazolone and esterification of the peptide, and liberation of the C-terminal amino acid with a vapor of 5% PFPA in methanol (ethanol) soln. at 5.degree.C for 5 min; and (3) hydrolysis of the peptide ester with 20% DMAE aq. solns. at 60.degree.C for 10 min. And the products are ready to the next step reaction.

L35 ANSWER 18 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:702370 HCAPLUS

DOCUMENT NUMBER: 128:32037

TITLE: **Identification** of the Components of Simple Protein Mixtures by High-Accuracy **Peptide Mass** Mapping and Database Searching

AUTHOR(S): Jensen, Ole N.; Podtelejnikov, Alexandre V.; Mann, Matthias

CORPORATE SOURCE: Protein Peptide Group, European Molecular Biology Laboratory (EMBL), Heidelberg, D-69117, Germany

SOURCE: Anal. Chem. (1997), 69(23), 4741-4750  
CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB **Peptide mass** mapping by matrix-assisted laser desorption/ionization (MALDI) followed by database searching with the set of measured **peptide** masses is now a powerful method for the **identification** of pure **proteins**. **Protein** mixts.-such as frequently occur due to comigration in polyacrylamide gel bands-have hitherto required **protein** sequencing. Here we demonstrate that such **protein** bands can also be analyzed by **peptide mass** mapping alone. Database searching with the complete list of **peptide** masses detd. by delayed-extn. MALDI **mass spectrometry** with a mass error of less than 30 ppm retrieves the most prominent **protein** in a mixt. In a second step, the **protein identity** is further confirmed by matching as many of the measured **peptide** masses as possible to the retrieved **amino acid** sequence. **Peptide** masses remaining after this "pass search" are searched again to **identify** the next component in the **protein** mixt. This iterative process is repeated until all major ion signals are accounted for. **Protein** mixts. consisting of two or more individual components in a single gel band can be analyzed, further increasing the general applicability of MALDI **peptide** mapping for **protein identification**.

L35 ANSWER 19 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:674722 HCAPLUS

DOCUMENT NUMBER: 127:343409

TITLE: Emerging tandem **mass spectrometry** techniques for the rapid **identification** of **proteins**

AUTHOR(S): Dongre, Ashok R.; Eng, Jimmy K.; Yates, John R., III

CORPORATE SOURCE: Department of Molecular Biotechnology, University of Washington, Seattle, WA, 98195, USA

SOURCE: Trends Biotechnol. (1997), 15(10), 418-425

CODEN: TRBIDM; ISSN: 0167-7799

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 68 refs. State-of-the-art techniques such as liq.-chromatog./electrospray-ionization tandem **mass spectrometry** have, in conjunction with database-searching computer algorithms, revolutionized the anal. of biochem. species from complex biol. mixts. With these techniques, it is now possible to perform high-throughput **protein identification** at picomolar-to-subpicomolar levels from **protein** mixts. This article provides an overview of the techniques and methods. available for the structural elucidation and **identification** of **proteins** and **peptides** from complex biol. samples.

L35 ANSWER 20 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:462934 HCAPLUS

DOCUMENT NUMBER: 127:187662

TITLE: Novel techniques for **identification** and characterization of proteins loaded on gels in femtomol amounts



AUTHOR(S): Gevaert, Kris; De Mol, Hans; Verschelde, Jean-Luc; Van Damme, Jozef; De Boeck, Stefaan; Vandekerckhove, Joel  
CORPORATE SOURCE: Flanders Interuniversity Institute for Biotechnology, Department of Biochemistry, Faculty of Medicine, Universiteit Gent, Belg.  
SOURCE: J. Protein Chem. (1997), 16(5), 335-342  
CODEN: JPCHD2; ISSN: 0277-8033  
PUBLISHER: Plenum  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A combination of techniques is presented allowing gel-purified **protein identification** in the femtomol range using matrix-assisted-laser-desorption-ionization **mass spectrometry**. The **proteins** are detected in the primary gel by sensitive neg. staining procedure, transferred, and concd. in a secondary gel matrix. There, they are digested in the presence of H<sub>2</sub> 180 and their sequences are predicted (1) by **peptide mass** fingerprinting, (2) by comparing the post-source-decay (PSD) spectra with theor. spectra of candidate isobaric **peptides** using a computer algorithm called MassFrag, and (3) by a manual readout of the 180/160-labeled fragmentation ions in the PSD spectra.

L35 ANSWER 21 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:336646 HCAPLUS  
DOCUMENT NUMBER: 127:62749  
TITLE: A two-dimensional gel database of human colon carcinoma proteins  
AUTHOR(S): Ji, Hong; Reid, Gavin E.; Moritz, Robert L.; Eddes, James S.; Burgess, Antony W.; Simpson, Richard J.  
CORPORATE SOURCE: Joint Protein Structure Laboratory, Ludwig Institute Cancer Research (Melbourne Branch) and Walter and Eliza Hall Medical Research, Parkville, Australia  
SOURCE: Electrophoresis (1997), 18(3-4), 605-613  
CODEN: ELCTDN; ISSN: 0173-0835  
PUBLISHER: VCH  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The master two-dimensional gel database of human colon carcinoma cells currently lists cellular **proteins** from normal crypts and the colorectal cancer cell lines LIM 1863, LIM 1215 and LIM 1899 (Ward et al., 1990; Ji et al., 1994). Updated 2-dimensional electrophoretic (2-DE) maps of cellular **proteins** from LIM 1215 cells acquired under both nonreducing and reducing conditions are presented. Fifteen cellular **proteins** are identified in the reducing 2-DE gel map and 7 in the nonreducing gel map, along with a tabular listing of their Mr/pI loci and mode of **identification**. We also include our **mass spectrometry**-based procedures for **identifying** 2-DE-resolved **proteins**. This procedure relies on a combination of capillary column (0.10-0.32 mm internal diam.) reversed-phase HPLC **peptide** mapping of in-gel digested **proteins**, **peptide mass** fingerprinting, sequence anal. by either collision-induced dissochn. or post-source-decay fragmentation, and **protein identification** using available database search algorithms. These data, and descriptions of the

microtechniques employed in this lab. for **identifying** 2-DE resolved **proteins** can be accessed via the Internet URL:  
<http://www.ludwig.edu.au>.

L35 ANSWER 22 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:336147 HCAPLUS

DOCUMENT NUMBER: 127:62707

TITLE: Probing **protein** function using a combination of gene knockout and **proteome** analysis by **mass spectrometry**

AUTHOR(S): Dainese, Paola; Staudenmann, Werner; Quadroni, Manfredo; Korostensky, Chantal; Gonnet, Gaston; Kertesz, Michael; James, Peter

CORPORATE SOURCE: Protein Chemistry Laboratory, Swiss Federal Institute Technology, ETH-Zentrum, Zurich, Switz.

SOURCE: Electrophoresis (1997), 18(3-4), 432-442  
CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: VCH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Recently the detn. of the genome sequences of three prokaryotes (Haemophilus influenzae, Methanococcus jannaschii and Mycoplasma genitalium) as well as the first eucaryotic genome (Saccharomyces cerevisiae) were completed. Between 40-60% of the genes were found to code for **proteins** to which no function could be assigned. We describe an approach which combines **proteome** anal. (mapping of expressed **proteins** isolated by two-dimensional polyacrylamide gel electrophoresis to the genome) with genetic manipulations to study the complex pattern of **protein** regulation occurring in Escherichia coli in response to sulfate starvation. We have previously described the upregulation of eight spots on two-dimensional (2-D) gels in response to sulfate starvation and the assignment of six of these to entries in the E. coli genome sequence (Quadroni et al., Eur. J. Biochem. 1996, 239, 773-781). Here we describe the **identification** of the remaining two **proteins** which are encoded in a sulfate-controlled operon in the 21.5' region of the E. coli genome. Upregulated **protein** spots were cut from multiple 2-D gels collected and run on a modified funnel gel to conc. the **proteins** and remove the sodium dodecyl sulfate before digestion. The **peptide** masses obtained from the digests were used to search the SwissProt database or a six-frame translation of the EMBL DNA database using a **peptide mass** fingerprinting algorithm. A digest can be reanalyzed after deuterium exchange to obtain a second, orthogonal data set to increase the confidence level of **protein identification**. The digests of the remaining unidentified **proteins** were used for **peptide** fragment generation using either post-source decay in a matrix-assisted laser desorption ionization (MALDI) time-of-flight **mass spectrometer** or collision-induced dissociation (CID) coupled **mass spectrometry** (MS/MS) with triple stage quadrupole or ion trap **mass spectrometers**. The spectra were used as **peptide** fragment fingerprints to search the SwissProt and EMBL databases.

L35 ANSWER 23 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:335482 HCAPLUS  
DOCUMENT NUMBER: 127:62733  
TITLE: **Identification of mouse liver proteins on two-dimensional electrophoresis gels by matrix-assisted laser desorption/ionization mass spectrometry of in situ enzymic digests**  
AUTHOR(S): O'Connell, Kathy L.; Stults, John T.  
CORPORATE SOURCE: Protein Chemistry Department, Genentech, Inc., South San Francisco, CA, USA  
SOURCE: Electrophoresis (1997), 18(3-4), 349-359  
CODEN: ELCTDN; ISSN: 0173-0835  
PUBLISHER: VCH  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A no. of **proteins** from a silver-stained two-dimensional (2-D) electrophoresis gel of mouse liver whole-cell lysate were **identified by peptide mass** mapping and sequence database searching. The excised **protein** spots were processed by in situ redn. and alkylation, followed by Lys-C digestion. The masses of the resulting **peptide** mixts. were measured with a matrix-assisted laser desorption/ionization (MALDI) reflection-time-of-flight **mass spectrometer**. These masses were used successfully to search a **protein** sequence database. Optimized silver staining and digestion protocols allowed **proteins** to be **identified** routinely at the low picomole level. The high mass accuracy and resolu. provided by delayed extn. were important for high specificity in the database search. Fragment ion data obtained by MALDI post-source decay (PSD) measurements not only provided confirmation of **peptide identification**, but could be used to **identify** the **protein** from a single **peptide** without spectral interpretation.

L35 ANSWER 24 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:20403 HCAPLUS  
DOCUMENT NUMBER: 126:56979  
TITLE: **Identification of proteins of the yeast protein map using genetically manipulated strains and peptide-mass fingerprinting**  
AUTHOR(S): Sagliocco, Francis; Guillemot, Jean-Claude; Monribot, Christelle; Capdevielle, Joel; Perrot, Michel; Ferran, Edgardo; Ferrara, Pascual; Boucherie, Helian  
CORPORATE SOURCE: CNRS, Institut de Biochimie et Genetique Cellulaires, Bordeaux, 33077, Fr.  
SOURCE: Yeast (1996), 12(15), 1519-1533  
CODEN: YESTE3; ISSN: 0749-503X  
PUBLISHER: Wiley  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB In this study we used genetically manipulated strains to **identify polypeptide** spots of the **protein** map of *Saccharomyces cerevisiae*. Thirty-two novel **polypeptide** spots were **identified** using this strategy. They corresponded to the product of 23 different genes. We also explored the possibilities of using

**peptide-mass** fingerprinting for the **identification** of **proteins** sepd. on our gels. According to this strategy, **proteins** contained in spots are digested with trypsin and the masses of generated **peptides** are detd. by matrix-assisted laser desorption-ionization **mass spectrometry** (MALDI-MS). The **peptide** masses are then used to search a yeast **protein** database for **proteins** that match the exptl. data. Application of this strategy to previously **identified polypeptide** spots gave evidence of the feasibility of this approach. We also report predictions on the **identities** of nine u MALDI-MS.

L35 ANSWER 25 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:746783 HCAPLUS

DOCUMENT NUMBER: 126:101318

TITLE: Linking genome and **proteome** by **mass spectrometry**: large-scale

**identification** of yeast **proteins** from two dimensional gels

AUTHOR(S): Shevchenko, Andrej; Jensen, Ole N.; Podtelejnikov, Alexandre V.; Sagliocco, Francis; Wilm, Matthias; Vorm, Ole; Mortensen, Peter; Shevchenko, Anna; Boucherie, Helian; Mann, Matthias

CORPORATE SOURCE: Peptide Protein Group, European Mol. Biol. Lab., Heidelberg, 69012, Germany

SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1996), 93(25), 14440-14445

CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The function of many of the uncharacterized open reading frames discovered by genomic sequencing can be detd. at the level of expressed gene products, the **proteome**. However, **identifying** the cognate gene from minute amts. of **protein** has been one of the major problems in mol. biol. Using yeast as an example, we demonstrate here that **mass spectrometric protein identification** is a general soln. to this problem given a completely sequenced genome. As a first screen, our strategy uses automated laser desorption ionization **mass spectrometry** of the **peptide** mixts. produced by in-gel tryptic digestion of a **protein**. Up to 90% of **proteins** are **identified** by searching sequence data bases by lists of **peptide** masses obtained with high accuracy. The remaining **proteins** are **identified** by partially sequencing several **peptides** of the unsepd. mixt. by nanoelectrospray tandem **mass spectrometry** followed by data base searching with multiple **peptide** sequence tags. In blind trials, the method led to unambiguous **identification** in all cases. In the largest individual **protein identification** project to date, a total of 150 gel spots - many of them at subpicomole amts. - were successfully analyzed, greatly enlarging a yeast two-dimensional gel data base. More than 32 **proteins** were novel and matched to previously uncharacterized open reading frames in the yeast genome. This

study establishes that **mass spectrometry** provides the required throughput, the certainty of **identification**, and the general applicability to serve as the method of choice to connect genome and **proteome**.

L35 ANSWER 26 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:659661 HCAPLUS

DOCUMENT NUMBER: 126:31620

TITLE: Search of sequence databases with uninterpreted high-energy collision-induced dissociation spectra of peptides

AUTHOR(S): Yates, John R., III; Eng, Jimmy K.; Clauser, Karl R.; Burlingame, Alma L.

CORPORATE SOURCE: Dep. Mol. Biotechnol., Univ. Washington, Seattle, WA, USA

SOURCE: J. Am. Soc. Mass Spectrom. (1996), 7(11), 1089-1098  
CODEN: JAMSEF; ISSN: 1044-0305

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The utility of the SEQUEST computer algorithm was broadened to permit correlation of uninterpreted high-energy collision-induced dissociation spectra of **peptides** with all sequences in a database. SEQUEST now allows for the addition of fragment ion types observed under high-energy conditions. Spectra were analyzed from **peptides** isolated following trypsin digestion of 13 **proteins**. SEQUEST ranked the correct sequence first for 90% (18/20) of the spectra in searches of the OWL database, without constraint by enzyme cleavage specificity or species of origin. All false-positives were flagged by the scoring system. SEQUEST searches databases for sequences that correspond to the precursor ion mass  $\pm 0.5$  u. Preliminary ranking of the top 500 candidates is done by calculation of fragment ion masses for each sequence, and comparison to the measured ion masses on the basis of ion series continuity, summed ion intensity, and immonium ion presence. Final ranking is done by construction of model spectra for the 500 candidates and constructing/performing of a cross-correlation analysis with the actual spectrum. Given the need to relate mounting genome sequence information with corresponding suites of **proteins** that comprise the cellular molecular machinery, tandem **mass spectrometry** appears destined to play the leading role in accelerating **protein identification** on the large scale required.

L35 ANSWER 27 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:658446 HCAPLUS

DOCUMENT NUMBER: 126:44592

TITLE: **Protein identification** by solid phase microextraction-capillary zone electrophoresis-microelectrospray-tandem **mass spectrometry**

AUTHOR(S): Figeys, Daniel; Ducret, Axel; Yates, John R., III; Aebersold, Ruedi

CORPORATE SOURCE: Department Molecular Biotechnology, Univ. Washington, Seattle, WA, 98195-7730, USA

SOURCE: Nat. Biotechnol. (1996), 14(11), 1579-1583

CODEN: NABIF9; ISSN: 1087-0156

PUBLISHER: Nature Publishing Co.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe an anal. system for the rapid **identification** of **proteins** by correlation of tandem **mass spectra** with **protein** sequence databases. The system consists of an integrated solid-phase microextn./capillary zone electrophoresis **peptide** sepn. device that is connected through a microelectrospray ion source to a tandem **mass spectrometer**. The limits of detection are 660 amol of sample at a concn. limit of <33 amol/.mu.L for **peptide mass** measurement, and <10 fmol of sample, at a concn. limit of <300 amol/.mu.L for **peptide** anal. by collision-induced dissocn. By using this system, we **identified** low-nanogram amts. of yeast **proteins** sepd. by high-resoln. 2-dimensional gel electrophoresis.

L35 ANSWER 28 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:593250 HCAPLUS

DOCUMENT NUMBER: 125:269426

TITLE: The **identification** of electrophoretically separated proteins by **peptide mass** fingerprinting

AUTHOR(S): Cottrell, John S.; Sutton, Chris W.

CORPORATE SOURCE: Finnigan MAT Ltd., Hemel Hempstead/Hertfordshire, UK

SOURCE: Methods Mol. Biol. (Totowa, N. J.) (1996), 61(Protein and Peptide Analysis by Mass Spectrometry), 67-82

CODEN: MMBIED; ISSN: 1064-3745

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review and discussion with 28 refs. about the principles and use of the title method to **identify proteins** for which sequences are already known. In a general approach, a **protein** is digested by a proteolytic enzyme, and the resulting digest is analyzed by **mass spectrometry** with matrix-assisted laser desorption/ionization or electrospray ionization. The mass values then are compared with a database of **peptide mass** values, calcd. by applying the enzyme cleavage rules to the entries in one of the major collections of sequence data. By using a scoring algorithm, the closest match or matches are **identified**. **Mass spectrometric** anal. might take 5-10 min/sample, whereas the search itself takes 2 min at most, and under best conditions, substantially <1 pmol of sample is needed for **mass spectrometric** anal.

L35 ANSWER 29 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:338663 HCAPLUS

DOCUMENT NUMBER: 125:79577

TITLE: Application of combined **mass spectrometry** and partial **amino acid** sequence to the **identification** of gel-separated **proteins**

AUTHOR(S): Patterson, Scott D.; Thomas, Didier; Bradshaw, Ralph A.

CORPORATE SOURCE: Amgen Inc., Thousand Oaks, CA, USA

SOURCE: Electrophoresis (1996), 17(5), 877-891

CODEN: ELCTDN; ISSN: 0173-0835

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The combined use of **peptide mass** information with **amino acid** sequence information derived by chem. sequencing or **mass spectrometry** (MS)-based approaches provides a powerful means of **protein identification**. We have used a two-part strategy to **identify proteins** from nerve growth factor (NGF)-stimulated rat adrenal pheochromocytoma cell line PC-12 cell lysates that assoc. with the adaptor **protein Shc** (Shc homologous and collagen **protein**). Initial expts. with metabolically radiolabeled cell exts. sepd. by SDS-PAGE revealed a no. of **proteins** that coimmunoptd. with anti-Shc antibody compared with control (unstimulated) cell exts. The expt. was scaled up and cell lysate from NGF-stimulated PC-12 cells was applied to a glutathione-S-transferase (GST)-Shc affinity column, eluted, sepd. by SDS-PAGE and blotted to Immobilon-CD. The blotted **proteins** were proteolytically digested in situ, and the masses obtained from the extd. **peptides** were used in a **peptide-mass** search program in an attempt to **identify** the **protein**. Even if a strong candidate was found using this search, an addnl. step was preformed to confirm, the **identification**. The mixts. were fractionated by reversed-phase high-performance liq. chromatog. (RP-HPLC) and subjected to chem. sequencing to obtain (partial) sequence information, or post-source decay (PSD-) matrix-assisted laser-desorption ionization (MALDI)-MS to obtain sequence-specific fragment ions. This data was used in a **peptide-sequence** tag search to confirm the **identity** of the **proteins**. This combined approach allowed **identification** of four **proteins** of Mr 43000 to 2000000. In one case the **identified protein** clearly did not correspond to the radiolabeled band, but to a **protein** contaminant from the column. The advantages and pitfalls of the approach are discussed.

L35 ANSWER 30 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:260210 HCAPLUS

DOCUMENT NUMBER: 125:4871

TITLE: **Identification** of human myocardial **proteins** separated by two-dimensional electrophoresis with matrix-assisted laser desorption/ionization **mass spectrometry**

AUTHOR(S): Thiede, Bernd; Otto, Albrecht; Zimny-Arndt, Ursula; Mueller, Eva-Christina; Jungblut, Peter

CORPORATE SOURCE: Max-Delbrueck-Centrum Molekulare Medizin, Berlin, Germany

SOURCE: Electrophoresis (1996), 17(3), 588-99

CODEN: ELCTDN; ISSN: 0173-0835

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors optimized the measurement by MALDI-MS for the anal. of proteolytic digests of 2-DE-sepd. proteins. The direct anal. of peptide mixts. can be used for rapid and sensitive **protein**

**identification.** In some cases, more information about the protein can be obtained by sepg. the peptides by micro high-performance liq. chromatog. (HPLC) before employing MALDI-MS anal. More peptides are found than in the mixt., and comparison of HPLC patterns can reveal some differences to be post-translational modifications of proteins, even in the case of **identical peptide mass** fingerprints. Furthermore, carboxy-terminal sequencing by on-target carboxypeptidase P digestion can be used to confirm the obtained result without the need for more material. The search program FRAGFIT was modified and renamed FRAGMOD to include the modifications of methionine and tryptophan oxidn. and alkylation of cysteine by acrylamide into the mass search. By applying this procedure, 15 proteins were **identified**, among them two different putative phosphorylated forms of two proteins, a putative N-terminal blocking group and four dilated cardiomyopathy-assocd. proteins. The resulting approach for the **identification** may be used for large-scale investigations of 2-DE-sepd. proteins.

L35 ANSWER 31 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:236717 HCAPLUS

DOCUMENT NUMBER: 124:337035

TITLE: **Identification** of electroblotted proteins by **peptide mass** searching of a sequence database

AUTHOR(S): Stults, John T.; Henzel, William J.; Wong, Susan C.; Watanabe, Colin

CORPORATE SOURCE: Protein Chemistry Department, Genentech, Inc., South San Francisco, CA, 94080, USA

SOURCE: Mass Spectrom. Biol. Sci. (1996), 151-70. Editor(s): Burlingame, A. L.; Carr, Steven A. Humana: Totowa, N. J.

CODEN: 62PNAY

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The authors have developed a complimentary approach to **protein** sequencing that **identifies protein** by database searching on the basis of **peptide** masses. The **protein** is digested chem. or enzymically. A **mass spectrum** of the resulting **peptide** mixt. provides a **peptide-mass** fingerprint of the **protein**. A computer program performs a theor. digest of each **protein** in the database and attempts to match those mass lists to the measured **peptide mass** fingerprint within the constraints of the search.

L35 ANSWER 32 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:159516 HCAPLUS

DOCUMENT NUMBER: 124:255186

TITLE: Tracing cell signaling pathways using a combination of 2D gel electrophoresis and mass spectrometry

AUTHOR(S): Quadroni, Manfredo; Corti, Chantal; Staudenmann, Werner; Carafoli, Ernesto; James, Peter

CORPORATE SOURCE: Protein Chemistry and Biochemistry III Laboratories, Swiss Federal Institute Technology, Zurich, 8092, Switz.



SOURCE: Methods Protein Struct. Anal., [Proc. Int. Conf.],  
10th (1995), Meeting Date 1994, 187-93. Editor(s):  
Atassi, M. Zouhair; Appella, Ettore. Plenum: New  
York, N. Y.  
CODEN: 62LPAK

DOCUMENT TYPE: Conference  
LANGUAGE: English

AB The title topic is discussed with information on **protein**  
**identification** by mass mapping, cell signaling by calcium,  
application of **mass spectrometric** methods to cell  
signaling, etc.

L35 ANSWER 33 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:105659 HCAPLUS

DOCUMENT NUMBER: 124:197496

TITLE: **Identification** of proteins from  
two-dimensional electrophoresis gels by  
**peptide mass** fingerprinting

AUTHOR(S): Arnott, David P.; Henzel, William J.; Stults, John T.  
CORPORATE SOURCE: Protein Chem. Dep., Genentech, Inc., San Francisco,  
CA, 94080, USA

SOURCE: ACS Symp. Ser. (1996), 619(Biochemical and  
Biotechnological Applications of Electrospray  
Ionization Mass Spectrometry), 226-43  
CODEN: ACSMC8; ISSN: 0097-6156

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB As part of a project to **identify** factors involved in congestive  
heart failure, differences in **protein** expression levels between  
normal and enlarged (hypertrophic) heart cells were **identified**.  
In initial expts. two-dimensional gel electrophoresis was used to sep. the  
**proteins** from normal neonatal rat cardiac myocytes. The  
**proteins** were electrobotted to a membrane and **identified**  
by staining. **Proteins** of interest were cleaved into  
**peptides** with an in situ enzymic digestion method. The masses of  
the **peptides** were det. dby capillary high performance liq.  
chromatog. electrospray ionization **mass spectrometry**  
and, when possible, partial sequences were obtained by subsequent liq.  
chromatog. tandem **mass spectrometry** (LC-MS/MS) expts.  
These data were used to search a **protein** sequence database with  
the program FRAGFIT. The program theor. cleaves each **protein** in  
the database. By comparison of the exptl.-detd. **peptide** masses  
and the theor. masses, the program **identifies** the  
**protein** if it exists in the database. A partial sequence from the  
LC-MS/MS expt. was used to increase the specificity of the search. With  
this approach, eight **proteins** present in low picomole quantities  
on 2-D gels from cardiac myocytes have been **identified**, with 100  
fmol or less of each **peptide** component required for the  
**mass spectral** expts.

L35 ANSWER 34 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:60663 HCAPLUS

DOCUMENT NUMBER: 124:140182

TITLE: **Peptide-mass** profiles of

polyvinylidene difluoride-bound **proteins** by matrix-assisted laser desorption/ionization time-of-flight **mass spectrometry** in the presence of nonionic detergents

AUTHOR(S): Gharahdaghi, Farzin; Kirchner, Michele; Fernandez, Joseph; Mische, Sheenah M.

CORPORATE SOURCE: DNA Technol. Cent., Rockefeller Univ. Protein, New York, NY, 10021, USA

SOURCE: Anal. Biochem. (1996), 233(1), 94-9  
CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization time-of-flight **mass spectrometry** (MALDI-TOF MS), in conjunction with enzymic digestion of **proteins** and mol. wt. search of **peptide-mass** database is a powerful technique for **peptide/protein identification**. Ideally, **peptide** mixts. should be compatible with both MALDI-TOF and microsequencing. In the lab., enzymic digestion and extn. of **peptides** from polyvinylidene difluoride (PVDF)-bound **proteins** is performed in the presence of nonionic detergents. However, nonionic detergents have been shown to cause signal suppression in MALDI-TOF anal. This study demonstrates that by using a modified matrix soln., **peptide-mass** fingerprinting of PVDF-bound **proteins** by MALDI-TOF can be obtained in the presence of nonionic detergents such as hydrogenated Triton X-100 (RTX-100), octylglucopyranoside, and Tween 20.

L35 ANSWER 35 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:719628 HCAPLUS

DOCUMENT NUMBER: 123:107010

TITLE: Matrix-assisted laser-desorption/ionization **mass spectrometric** approaches for the **identification** of gel-separated **proteins** in the 5-50 pmol range

AUTHOR(S): Patterson, Scott D.

CORPORATE SOURCE: Amgen Inc., Thousand Oaks, CA, USA

SOURCE: Electrophoresis (1995), 16(7), 1104-14

CODEN: ELCTDN; ISSN: 0173-0835

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ability to **identify** and characterize low picomole quantities of gel-sepd. **proteins** has greatly benefited from recent advancements in **mass spectrometric** anal. methods, particularly **peptide-mass** search routines. The authors are investigating the use of matrix-assisted laser desorption/ionization **mass spectrometry** (MALDI-MS) to gain as much mass information as possible from a single gel-sepd. **protein** species. This report details results obtained from one-dimensional SDS-PAGE sepns., under nonreducing conditions, of known quantities of three **proteins**, followed by blotting to Immobilon-CD. Three methods were used to obtain MALDI-MS data from a single blotted **protein** band: (1) direct MALDI-MS of .apprx.10% of the band, (2) CNBr cleavage of another .apprx.10% of the band, and (3) enzymic (**endoproteinase** Lys-C) digestion of the remaining

.apprx.70-80% of the band followed by MALDI-MS. At the level of 50 pmol of **protein** loaded onto the gel, data was obtained from all three approaches. At levels down to 5 pmol of **protein** loaded onto the gel, MALDI-MS data was obtained from the latter two methods, CNBr and Lys-C digestions, but not direct MALDI-MS. Sufficient **peptide** masses were obtained from the 5 pmol loads to **identify** two of the three test **proteins** using four mass search programs. Only limited **peptide mass** data was obtained from fetuin, a sialylated **glycoprotein** with six disulfides and no methionines, but it was **identified**.

L35 ANSWER 36 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:707889 HCAPLUS

DOCUMENT NUMBER: 123:105683

TITLE: Reactivation of phosphorylated actin depolymerizing factor and **identification** of the regulatory site

AUTHOR(S): Agnew, Brian J.; Minamide, Laurie S.; Bamburg, James R.

CORPORATE SOURCE: Dep. Biochem. Mol. Biol., Colorado State Univ., Fort Collins, CO, 80523, USA

SOURCE: J. Biol. Chem. (1995), 270(29), 17582-7

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Actin depolymg. factor (ADF) occurs naturally in two forms, one of which contains a phosphorylated Ser and does not bind G-actin or depolymerize F-actin. Removal of this phosphate in vitro by alk. phosphatase restores full F-actin depolymg. activity. To **identify** the phosphorylation site, [32P]pADF was purified and digested with **endoproteinase** Lys-C. The digest contained only one 32P-labeled **peptide**. Further digestion with **endoproteinase** Asp-N and **mass spectrometric** anal. showed that this **peptide** came from the N terminus of ADF. Alk. phosphatase treatment of one Asp-N **peptide** (**mass** 753) converted it to a **peptide** of mass 673, demonstrating that this **peptide** contains the phosphate group. Tandem **mass spectrometric** sequence anal. of this **peptide** **identified** the phosphorylated Ser as the encoded Ser3 (Ser2 in the processed **protein**). HeLa cells, transfected with either chick wild-type ADF cDNA or a cDNA mutated to code for Ala in place of Ser24 or Thr25, express and phosphorylate the exogenous ADF. Cells also expressed high levels of mutant ADF when Ser3 was deleted or converted to either Ala or Glu. However, none of these mutants was phosphorylated, confirming that Ser3 in the encoded ADF is the single in vivo regulatory site.

L35 ANSWER 37 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:482008 HCAPLUS

DOCUMENT NUMBER: 122:209020

TITLE: Recognition of the Carboxy-Terminal Peptide in Cyanogen Bromide Digests of Proteins

AUTHOR(S): Murphy, Constance M.; Fenselau, Catherine

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, MD, 21228,

USA  
SOURCE: Anal. Chem. (1995), 67(9), 1644-5  
CODEN: ANCHAM; ISSN: 0003-2700  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Recognition is based on **mass spectrometric** anal. of the **peptide** products before and after reaction with acidic methanol. **Peptides** generated from internal positions in the **protein** are terminated by homoserine lactone, which undergoes methanolysis to add 32 mass units. The **peptide** contg. the original carboxyl terminus is converted to a Me ester, with a mass increment of 14 Da.

L35 ANSWER 38 OF 48 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1994:647335 HCAPLUS  
DOCUMENT NUMBER: 121:247335  
TITLE: **Protein identification in DNA databases by peptide mass fingerprinting**  
AUTHOR(S): James, Peter; Quadroni, Manfredo; Carafoli, Ernesto; Gonnet, Gaston  
CORPORATE SOURCE: Dep. Biology, Swiss Federal Institute Technology, Zurich, 8092, Switz.  
SOURCE: Protein Sci. (1994), 3(8), 1347-50  
CODEN: PRCIEI; ISSN: 0961-8368  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Proteins can be **identified** using a set of peptide fragment wts. produced by a specific digestion to search a protein database in which sequences have been replaced by fragment wts. calcd. for various cleavage methods. We present a method using multidimensional searches that greatly increases the confidence level for **identification**, allowing DNA sequence databases to be examd. This method provides a link between 2-dimensional gel electrophoresis protein databases and genome sequencing projects. Moreover, the increased confidence level allows unknown proteins to be matched to expressed sequence tags, potentially eliminating the need to obtain sequence information for cloning. Database searching from a mass profile is offered as a free service by an automatic server at the Swiss Federal Institute of Technol. (ETH), Zurich. For information, send an electronic message to the address cbrg@inf.ethz.ch with the line: help mass search, or help all.

L35 ANSWER 39 OF 48 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1994:625756 HCAPLUS  
DOCUMENT NUMBER: 121:225756  
TITLE: Microbore reversed-phase high-performance liquid chromatographic purification of **peptides** for combined chemical sequencing-laser-desorption **mass spectrometric** analysis  
AUTHOR(S): Elicone, Christopher; Lui, Mary; Geromanos, Scott; Erdjument-Bromage, Hediye; Tempst, Paul  
CORPORATE SOURCE: Molecular Biology Program and Protein Chemistry Laboratory, Memorial Sloan-Kettering Cancer Center (Box 137), 1275 York Avenue, New York, NY, 10021, USA

SOURCE: J. Chromatogr., A (1994), 676(1), 121-37  
CODEN: JCRAEY

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An optimized microbore RP-HPLC system (1.0 mm I.D. columns) for the purifn. of low picomole amts. (<5 pmol) of **peptides** is described. It is comprised of com. available columns, instrument components and parts. These were selected on the basis of a comparative evaluation and to yield the highest resoln. and most efficient peak collection. The sensitivity of this system equals, probably surpasses, that of advanced chem. microsequencing for which 2-4 pmol of **peptide** are minimally required. As an automated sequencer cannot be "online" connected with a micro-preparative HPLC system, fractions must be collected and transferred. With a typical flow of 30 .mu.L, efficient manual collection is possible and fractions (about 20 .mu.L in vol.) can still be handled without unacceptable losses, albeit with great precaution. Furthermore, major difficulties were encountered to efficiently and quant. load low- or sub-picomole amts. of **peptide** mixts. onto the RP-HPLC column for sepn. Discipline and rigorous adherence to sample handling protocols are thus on order when working at those levels of sensitivity. With adequate instrumentation and handling procedures in place, we demonstrate that low picomole amts. of **peptides** can now be routinely prepd. for anal. by combined Edman-chem. sequencing-matrix-assisted laser-desorption **mass spectrometry** (MALDI-MS). The integrated method was applied to covalent structural characterization of minute quantities of a gel-purified **protein** of known biol. function but unknown **identity**. The results allowed unambiguous **identification** and illustrated the power of MALDI-MS-aided interpretation of chem. sequencing data: accurate **peptide** masses were crucial for (i) confirmation of the results, (ii) deconvolution of mixed sequences, (iii) proposal of complete structures on the basis of partial sequences, and (i.v.) confirmation of **protein identification** (obtained by database search with a single, small stretch of **peptide** sequence) by "mass matching" of several more **peptides** with predicted proteolytic fragments.

L35 ANSWER 40 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1994:574143 HCAPLUS

DOCUMENT NUMBER: 121:174143

TITLE: **Protein identification by peptide mass fingerprinting**

AUTHOR(S): Cottrell, John S.

CORPORATE SOURCE: Finnigan MAT Ltd., Hemel Hempstead, UK

SOURCE: Pept. Res. (1994), 7(3), 115-18, 120-4

CODEN: PEREEO; ISSN: 1040-5704

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 22 refs. on **protein identification** by **peptide mass** fingerprinting. This review aims to provide an overview of the technique, compare the different database matching algorithms which have been described in the literature, and discuss the practical and theor. factors which influence **identification** accuracy.

L35 ANSWER 41 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1994:318644 HCAPLUS

DOCUMENT NUMBER: 120:318644

TITLE: **Identification of transformation-sensitive proteins recorded in human two-dimensional gel protein databases by mass spectrometric peptide mapping alone**

AUTHOR(S): Rasmussen, Hanne H.; Mertz, Ejvind; Mann, Matthias; Roepstorff, Peter; Celis, Julio E.

CORPORATE SOURCE: Inst. Med. Biochem., Aarhus Univ., Aarhus, Den.

SOURCE: Electrophoresis (Weinheim, Fed. Repub. Ger.) (1994), 15(3-4), 406-16

DOCUMENT TYPE: CODEN: ELCTDN; ISSN: 0173-0835

LANGUAGE: Journal

AB A comprehensive human keratinocyte two-dimensional (2-D) gel **protein** database was established to study the expression levels and properties of the thousands of **proteins** that orchestrate various keratinocyte functions both in health and disease, cancer included. A major task in establishing such a database is to **identify** known **proteins** in the 2-D gel patterns as well as to reveal hitherto unknown **proteins**. To date, **protein identification** has been performed by one or a combination of the following methods: (1) comigration with known **proteins**, (2) Western blotting using specific antibodies, (3) microsequencing, and (4) vaccinia virus expression of full length cDNAs. Recently, the systematic **identification of proteins** has gained a new dimension with the advent of computer programs for searching **peptide** mol. mass databases with exptl. obtained **peptide mass** maps. Here the authors investigate this approach to **identify proteins** that are highly up- or down-regulated in simian virus SV40 transformed human keratinocytes (K14). **Peptide mass** maps of several **proteins**, including keratins 7, 8, 18, and 19 were obtained either by plasma desorption **mass spectrometry** (PDMS) anal. of HPLC-purified **peptides** or by matrix-assisted laser desorption/ionization **mass spectrometry** (MALDI-MS) of total digests. The results demonstrated that **peptide mass** maps can be used for a rapid and sensitive **protein identification** allowing fast screening of **proteins** recorded in 2-D gel databases. The **mass spectrometric** approach when combined with microsequencing strengthened **identification**, and added the possibility of full characterization of posttranslational modifications and sequence variations.

L35 ANSWER 42 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1994:318643 HCAPLUS

DOCUMENT NUMBER: 120:318643

TITLE: Two-dimensional electrophoretic analysis of **proteins** expressed by normal and cancerous human crypts: application of **mass spectrometry to peptide-mass**

fingerprinting  
AUTHOR(S): Ji, Hong; Whitehead, Robert H.; Reid, Gavin E.;  
Moritz, Robert L.; Ward, Larry D.; Simpson, Richard J.  
CORPORATE SOURCE: Jt. Protein Struct. Lab., Walter and Eliza Hall Inst.  
Med. Res., Parkville, Australia  
SOURCE: Electrophoresis (Weinheim, Fed. Repub. Ger.) (1994),  
15(3-4), 391-405  
CODEN: ELCTDN; ISSN: 0173-0835  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB **Protein** patterns of normal human colonic crypts, isolated from different regions of the large intestine, and several colorectal cancer cell lines were compared using two-dimensional electrophoresis gels (2-DE). As detected by intrinsic radiolabeling and Coomassie Brilliant Blue staining, the **protein** patterns for normal crypts isolated from the ascending, and descending, regions of the colon and the rectum, were almost (>95%) **identical**. While 75-80% of the **protein** spots from normal crypts and the colorectal cancer cell line (LIM 1863), a cell line that grows as organoids and differentiates spontaneously into crypt-like structures in vitro, can be matched, the relative expression levels of a large no. of **proteins** differ. At least 2 **protein** spots (undetectable in the **protein** pattern from normal cells), **proteins** a (Mr .apprx.18,000, pI 6.7-6.9) and b (Mr .apprx.24,000, pI 5.9-6.0), were detected in the 2-DE gel **protein** pattern in the 3 cells lines LIM 1863, LIM 1215, and LIM 1899. The **identity** of these **proteins** is not yet known and further studies are required before they can be considered as potential colon tumor markers. Approx. 60% of the cellular **proteins** from LIM 1215 cells, a colon carcinoma cell line that exhibits many properties assocd. with columnar cells, can be matched with LIM 1863 cells. The results presented here represent an initial phase in the authors' efforts to develop a comprehensive **protein** database for normal human colon cells and several colorectal cancer cell lines. While the authors' initial **protein identification** relied on microsequencing methodologies, the authors are presently evaluating **peptide-mass** fingerprinting, utilizing capillary reversed-phase HPLC, and electrospray **mass spectrometry**, as a means for rapid **identification** of **proteins** at subpicomole levels. Using this approach, **protein** #3 (Mr .apprx. 66,000, pI 6.2) was **identified** as heat shock **protein** 60 from as few as 7 **peptide** masses when they were screened against the mol. wt. search (MOWSE) **peptide-mass** database.

L35 ANSWER 43 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1994:3992 HCAPLUS

DOCUMENT NUMBER: 120:3992

TITLE: **Peptide mass** maps: A highly  
informative approach to **protein**  
**identification**

AUTHOR(S): Yates, John R., III; Speicher, Stephen; Griffin,  
Patrick R.; Hunkapiller, Tim

CORPORATE SOURCE: Sch. Med., Univ. Washington, Seattle, WA, 98195, USA  
SOURCE: Anal. Biochem. (1993), 214(2), 397-408

CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB A computer searching algorithm has been used to **identify** **protein** sequences in the **Protein** Information Resource (PIR) database with **peptide mass** information (mass map) obtained from proteolytic digests of **proteins** analyzed by microcapillary high-performance liq. chromatog. electrospray ionization **mass spectrometry**. A theor. anal. of the cytochrome c family demonstrates the ability to **identify protein** sequences in the PIR database with a high degree of accuracy using a set of six predicted tryptic **peptide** masses. This method was also applied to exptl. detd. **peptide** masses for a small GTP-binding **protein**, a **protein** from pig uterus, the human sex steroid binding **protein**, and a thermostable DNA polymerase. The results demonstrate that a set of obsd. masses which is less than 50% of the total no. of predicted masses can be used to **identify** a **protein** sequence in the database. For the anal. presented in this paper, a mass matching tolerance of 1 amu is used. Under these conditions, mass maps created by fast atom bombardment **mass spectrometry** and matrix-assisted laser desorption time-of-flight would also be applicable. In cases where multiple matches are obsd. or verification of the **protein identification** is needed, tandem **mass spectrometry** sequencing can be used to establish sequence similarity.

L35 ANSWER 44 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER:

1993:644768 HCAPLUS

DOCUMENT NUMBER:

119:244768

TITLE:

Rapid indentification of proteins by **peptide**  
-**mass** fingerprinting. [Erratum to document  
cited in CA119(15):155221x]

AUTHOR(S):

Pappin, D. J.; Hojrup, P.; Bleasby, A. J.

CORPORATE SOURCE:

Protein Sequencing Lab., Imp. Cancer Res. Fund,  
London, WC2A 3PX, UK

SOURCE:

Curr. Biol. (1993), 3(7), 487  
CODEN: CUBLE2; ISSN: 0960-9822

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The errors were not reflected in the abstr. or the index entries.

L35 ANSWER 45 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER:

1993:555221 HCAPLUS

DOCUMENT NUMBER:

119:155221

TITLE:

Rapid indentification of proteins by **peptide**  
-**mass** fingerprinting

AUTHOR(S):

Pappin, D. J. C.; Hojrup, P.; Bleasby, A. J.

CORPORATE SOURCE:

Protein Sequencing Lab., Imp. Cancer Res. Fund,  
London, WC2A 3PX, UK

SOURCE:

Curr. Biol. (1993), 3(6), 327-32  
CODEN: CUBLE2; ISSN: 0960-9822

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The authors report the development of the mol. wt. search (MOWSE)



**peptide-mass** database at the SERC Daresbury Lab. Practical experience showed that sample proteins can be **identified** uniquely from as few as 3 or 4 exptl. detd. peptide masses when these are screened against a fragment database that is derived from >50,000 proteins. **Peptide-mass** fingerprints can prove as discriminating as linear peptide sequences but can be obtained in a fraction of the time using less protein. In many cases, this allows for a rapid **identification** of a sample protein before committing it to protein sequence anal. Fragment masses also provide information, at the protein level, that is complementary to the information provided by large-scale DNA sequencing or mapping projects.

L35 ANSWER 46 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1991:58326 HCAPLUS

DOCUMENT NUMBER: 114:58326

TITLE: Strategies for determination of disulfide bridges in **proteins** using plasma desorption **mass spectrometry**

AUTHOR(S): Soerensen, Hans Holmegaard; Thomsen, Johannes; Bayne, Stephen; Hoejrup, Peter; Roepstorff, Peter

CORPORATE SOURCE: Novo Nordisk A/S, Gentofte, DK-2820, Den.  
SOURCE: Biomed. Environ. Mass Spectrom. (1990), 19(11), 713-20  
CODEN: BEMSEN; ISSN: 0887-6134

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Disulfide bridges have been assigned in 3 different **proteins** by locating possible disulfide-linked **peptides** in enzymic digests of the **proteins** based on their mol. wt. detd. by plasma desorption **mass spectrometry**. Different strategies have been employed including in situ redn. of the nitrocellulose-bound **peptides** and confirmation of **peptide identify** by Me esterification reactions or Edman degradn. The latter was needed for **identification** of glycosylated disulfide-linked **peptides**. For insulins cleaved between cysteine residues in close proximity was not possible; but a combination of mol. mass information, enzymic cleavage with 2 different enzymes and sequence anal. including **identification** of diphenylthiohydantoin-cystine could ensure an unambiguous assignment of the disulfide bridges.

L35 ANSWER 47 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1987:632347 HCAPLUS

DOCUMENT NUMBER: 107:232347

TITLE: Structural analysis of **glycoproteins: identification** of carbohydrates and other posttranslational modifications by **mass spectrometry**

AUTHOR(S): Carr, Steven A.; Roberts, Gerald D.  
CORPORATE SOURCE: Dep. Anal., Phys. Struct. Chem., SmithKline and French Lab., Swedeland, PA, 19479, USA

SOURCE: Methods Protein Sequence Anal., [Proc. Int. Conf.], 6th (1987), Meeting Date 1986, 423-36. Editor(s): Walsh, Kenneth A. Humana: Clifton, N. J.  
CODEN: 56DFAZ

DOCUMENT TYPE: Conference; General Review

LANGUAGE: English  
AB A review with 33 refs. about some of the unique problems assocd. with structural characterization of **glycoproteins** and an anal. strategy utilizing fast-atom-bombardment **mass spectrometry** and biochem. manipulations for **identifying** sites of attachment of asparagine-linked carbohydrates, detg. the extent of glycosylation at specific sites and defining the compn. and heterogeneity of oligosaccharides from unique sites.

L35 ANSWER 48 OF 48 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1982:100377 HCAPLUS  
DOCUMENT NUMBER: 96:100377  
TITLE: 252Californium plasma desorption mass spectrometry  
AUTHOR(S): Macfarlane, Ronald D.  
CORPORATE SOURCE: Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA  
SOURCE: Biomed. Mass Spectrom. (1981), 8(9), 449-53  
CODEN: BMSYAL; ISSN: 0306-042X  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB The basic principles of 252Cf plasma desorption mass spectrometry are presented, with examples of its application including the **identification** of nonvolatile marine toxins (including the red tide toxin). A new variation in mass spectrometry, a study of time-dependent effects, is presented; it is a technique which can be used to follow dynamic changes as a result of chem. reactions occurring in a sample at room temp. This is possible in 252Cf plasma desorption mass spectrometry because the sample is conserved during the anal.

=> d stat que  
L4 2842848 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR AMIN? OR PROTEOME?)  
L5 224579 SEA FILE=HCAPLUS (MASS(W)SPECTR?)  
L6 26790 SEA FILE=HCAPLUS L4(L)L5  
L14 1924052 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR PROTEOME?)  
L27 1886 SEA FILE=HCAPLUS L14 (W)MASS  
L28 1074 SEA FILE=HCAPLUS L27 AND L6  
L30 436 SEA FILE=HCAPLUS L28 AND IDENT?  
L33 6258 SEA FILE=HCAPLUS L14 (W)IDENT?  
L34 115 SEA FILE=HCAPLUS L30 AND L33  
L35 48 SEA FILE=HCAPLUS L34 NOT (2001 OR 2000 OR 1999)/PY  
L36 18368 SEA FILE=HCAPLUS L14 AND L6  
L38 93 SEA FILE=HCAPLUS L36 AND INDEX  
L39 92 SEA FILE=HCAPLUS L38 NOT L35  
L40 65 SEA FILE=HCAPLUS L39 NOT (2001 OR 2000 OR 1999)/PY  
L41 4 SEA FILE=HCAPLUS L40 AND POLYPEPTIDE?  
L44 4 SEA FILE=HCAPLUS L28 AND L38  
L46 8 SEA FILE=HCAPLUS L41 OR L44

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L46 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:584259 HCAPLUS  
DOCUMENT NUMBER: 127:244507  
TITLE: **Proteome** analysis of *Spiroplasma melleiferum* (A56) and **protein** characterization across species boundaries  
AUTHOR(S): Cordwell, Stuart J.; Basseal, David J.; Humphery-Smith, Ian  
CORPORATE SOURCE: Center Proteome Research Gene-Product Mapping, National Innovation Center, Eveleigh, 1430, Australia  
SOURCE: Electrophoresis (1997), 18(8), 1335-1346  
CODEN: ELCTDN; ISSN: 0173-0835  
PUBLISHER: Wiley-VCH  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB *Spiroplasma melleiferum* (Class: Mollicutes) is a wall-less, helical bacterium with a genome of approx. 1460 kbp encoding 800 - 1000 gene-products. A two-dimensional electrophoresis gel ref. map of *S. melleiferum* was produced by Phoretix 2-D gel software anal. of eight high quality gels. The ref. map showed 456 silver-stained and replicated **protein spots**. 156 **Proteins** (34% of visible **protein spots**) from *S. melleiferum* were further characterized by one, or a combination, of the following: **amino acid anal.**, **peptide-mass** fingerprinting via matrix assisted laser desorption ionization-time of flight (MALDI-TOF) **mass spectrometry**, and N-terminal **protein** microsequencing. **Proteins** with close relationships to those previously detd. from other species were identified across species barriers. Thus, this study represents the first larger-scale anal. of a **proteome** based upon the attribution of predominantly "unique numerical parameters" for **protein** characterization across species boundaries, as opposed to a sequence-based approach. This approach allowed all database entries to be screened for homol., as is currently the case for studies based on nucleic acid or **protein** sequence information. Several **proteins** studied from this organism were identified as hypothetical, or having no close homolog already present in the databases. Gene-products from major families such as glycolysis, translation, transcription, cellular processes, energy metab., and **protein** synthesis were identified. Several gene-products characterized in *S. melleiferum* were not previously found in studies of the entire *Mycoplasma genitalium* and *Mycoplasma pneumoniae* (both closely related Mollicutes) genomes. The presence of such gene-products in *S. melleiferum* is discussed in terms of genome size as compared with the smallest known free-living organisms. Finally, the levels of expression of *S. melleiferum* gene-products were detd. with respect to total optical intensity assocd. with all visible **proteins** expressed in exponentially grown cells.

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L46 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1993:644768 HCAPLUS  
DOCUMENT NUMBER: 119:244768  
TITLE: Rapid indentification of **proteins** by

**peptide-mass** fingerprinting.  
[Erratum to document cited in CAl19(15):155221x]  
AUTHOR(S): Pappin, D. J.; Hojrup, P.; Bleasby, A. J.  
CORPORATE SOURCE: Protein Sequencing Lab., Imp. Cancer Res. Fund,  
London, WC2A 3PX, UK  
SOURCE: Curr. Biol. (1993), 3(7), 487  
CODEN: CUBLE2; ISSN: 0960-9822  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The errors were not reflected in the abstr. or the **index**  
entries.

L46 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1991:20437 HCAPLUS  
DOCUMENT NUMBER: 114:20437  
TITLE: MacProMass: a computer program to correlate  
**mass spectral** data to  
**peptide** and **protein** structures  
AUTHOR(S): Lee, Terry D.; Vemuri, Sunil  
CORPORATE SOURCE: Div. Immunol., Beckman Res. Inst., City of Hope,  
Duarte, CA, 91010, USA  
SOURCE: Biomed. Environ. Mass Spectrom. (1990), 19(11), 639-45  
CODEN: BEMSEN; ISSN: 0887-6134  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A program known as MacProMass has been written for Macintosh computers to  
assist in the anal. of **mass spectral** data of  
**peptides** and **proteins**. The program employs a user  
friendly, graphical interface and accommodates a variety of  
**protein** structures including cyclic **peptides** and  
multiple chain **proteins**. In addn. to mol. mass calcns. for pos.  
and neg. mol. ions, MacProMass also calcs. elemental compn., **amino**  
acid compn., isoelec. point, surface free energy, and HPLC **index**  
values for whole structures and **peptide** fragments resulting from  
enzymic or chem. degrdn. Users can program their own **amino acid**  
residues and terminal groups. In addn. to search routines for both mass  
and sequence, theor. fragment ions for **peptide mass**  
**spectra** can be calcd. Anal. of variant **proteins** is  
facilitated with a subroutine that systematically catalogs single  
**amino acid** substitutions that correspond to mass differences  
between obsd. and expected mol. ions. Interchain and intrachain disulfide  
bonds and other types of linkages are maintained throughout the chem. and  
enzymic degrdn. operations.

L46 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
ACCESSION NUMBER: 1990:441319 HCAPLUS  
DOCUMENT NUMBER: 113:41319  
TITLE: Effects of **peptide** hydrophobicity and charge  
state on molecular ion yields in plasma desorption  
**mass spectrometry**  
AUTHOR(S): Wang, Rong; Chen, Ling; Cotter, Robert J.  
CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205,  
USA  
SOURCE: Anal. Chem. (1990), 62(15), 1700-5

CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Plasma desorption **mass spectra** were obtained for a series of **peptides**, grouped in 4 mass ranges having approx. 9, 20, 30, and 40 **amino acid** residues. Within each group, the individual **peptides** differed in hydrophobicity, charge state, and retention time, as measured on a reversed-phase HPLC column. Comparison of the mol. ion intensities in the pos. ion **mass spectra** of **peptides** from each group showed a strong dependence upon hydrophobicity and no correlation with charge state. Plasma desorption **mass spectra** of mixts. of all the **peptides** within each mass range generally resulted in the desorption of a single residue and suppression of the ion signal from other components. In most cases, this could be correlated with hydrophobicity, as calcd. from the Bull and Breese **index** (Bull, H.B.; Breese, K., 1974); however, a better correlation existed when the results were compared with reversed-phase retention times. In general, the spectra of mixts. were not influenced by charge state (except in the absence of hydrophobic **peptides**), as the same components in each **peptide** mixt. produced the most abundant ions in both pos. and neg. ion spectra.

L46 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1986:549134 HCAPLUS

DOCUMENT NUMBER: 105:149134

TITLE: An approach towards the complete FAB analysis of enzymic digests of **peptides** and **proteins**

AUTHOR(S): Naylor, Stephen; Findeis, A. Frederick; Gibson, Bradford W.; Williams, Dudley H.

CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, CB2 1EW, UK  
SOURCE: J. Am. Chem. Soc. (1986), 108(20), 6359-63  
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A current limitation in the use of fast-atom-bombardment (FAB) **mass spectrometry** for mixt. anal. is that some components of the mixt., dissolved in matrixes such as glycerol, are not normally obsd. Three enzymic digestions (1 of a **polypeptide** and 2 of small **proteins**) were used to show that it is the hydrophilic **peptides** in a mixt. that are suppressed. By detn. of the FAB spectra of both pure hydrophilic and hydrophobic **peptides** and of mixts. of these, it is shown that (1) hydrophilic **peptides** alone give a relatively poor signal response and (2) hydrophilic **peptides** are further suppressed in the presence of hydrophobic **peptides** that initially occupy the surface of the matrix. A hydrophilicity/hydrophobicity **index** (.DELTA.F values) can be used to indicate which **peptide** may be suppressed. Suppression may be reduced by HPLC partial fractionation or the conversion of polar carboxyl groups to more hydrophobic ester derivs.

L46 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1984:2927 HCAPLUS

DOCUMENT NUMBER: 100:2927  
TITLE: **Amino acid sequence determination by gas chromatography-mass spectrometry of permethylated peptides.** The application of capillary columns  
AUTHOR(S): Rose, Keith; Bairoch, Amos; Offord, Robin E.  
CORPORATE SOURCE: Dep. Biochim. Med., CMU, Geneva, 1211, Switz.  
SOURCE: J. Chromatogr. (1983), 268(2), 197-206  
CODEN: JOCRAM; ISSN: 0021-9673  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The application of capillary columns to the detn. of the **amino acid sequence of proteins and polypeptides** by gas chromatog.-**mass spectrometry** (GC-MS) of partial hydrolyzates is described and discussed for the case of the N.alpha.,.epsilon.-trifluoroacetyl-N,O-permethyl derivs. Retention indexes are detd. with the aid of a computer program. The **mass spectra** of methionine enkephalin obtained by GC-MS on a packed and on a capillary column are presented and a retention **index** calcd. Amts. of deriv. corresponding to subnanomole amts. of **peptides** are sufficient to provide full **amino acid sequence information**. To assist in the assignment of retention indexes above 4400, a mixt. of n-alkanes from a com. source was characterized by GC-MS up to n-C54H110, and was found to contain material up to an expected C72H146.

L46 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1976:474449 HCAPLUS  
DOCUMENT NUMBER: 85:74449  
TITLE: **Amino acid sequencing by gas chromatography-mass spectrometry using trifluoro-dideuteroalkylated peptide derivatives.** C. The primary structure of the carboxypeptidase inhibitor from potatoes  
AUTHOR(S): Nau, Heinz; Biemann, K.  
CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, Mass., USA  
SOURCE: Anal. Biochem. (1976), 73(1), 175-86  
CODEN: ANBCA2  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The carboxypeptidase inhibitor from potatoes was used to demonstrate the utility of gas chromatog.-**mass spectrometry** for the detn. of the primary structure of such large **polypeptides**. Two mixts. of **oligopeptide** fragments, obtained by limited acid hydrolysis and enzymic digestion of this **polypeptide**, were transformed into the corresponding mixts. of O-trimethylsilylated trifluoro-dideuteroethyl polyamino alcs. which were then analyzed by gas chromatog.-**mass spectrometry**. The resulting **mass spectral** and retention **index** data allowed the identification of 61 **oligopeptide** fragments that were assembled by the computer by positioning all 39 **amino acid** residues in a unique sequence (with the exception of the assignment of the primary amide groups of Asn and Gln).

L46 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1974:92814 HCAPLUS

DOCUMENT NUMBER: 80:92814

TITLE: Computer-assisted assignment of retention indexes in gas chromatography-mass spectrometry and its application to mixtures of biological origin

AUTHOR(S): Nau, H.; Biemann, K.

CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, Mass., USA

SOURCE: Anal. Chem. (1974), 46(3), 426-34

CODEN: ANCHAM

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A program was written for the automatic assignment of the retention indexes of all components eluted during a gas chromatog.-**mass spectrometry**-computer expt. A set of 3 std. compds. (e.g. n-alkanes) is cojected with the sample into the gas chromatograph. The computer then identifies these compds. by their **mass spectral** characteristics and uses their positions to assign retention indexes for the entire gas chromatogram. The combination of these 2 sets of data that are structure specific and complementary, namely retention indexes and **mass spectra**, constitutes a most efficient and reliable approach to the identification of compds. Applications to the identification of drugs in body fluids of comatose patients as well as to the complete characterization of **amino acids** and **oligopeptides** in derivatized **polypeptide** hydrolyzates are presented. The **retention index** data provided by this program can be used for manual interpretation as well as for computer-assisted interpretation and search system.